Exchange interaction between magnetic impurities at surfaces

Eszter Simon

-PhD thesis booklet-

Eötvös Loránd University, Faculty of Natural Sciences

Supervisor: **Dr. Balázs Újfalussy**

Institute for Solid State Physics and Optics

Wigner Research Centre for Physics of H.A.S.

Doctoral School of Physics

Head of Doctoral School : Prof. Ferenc Csikor

Material Science and Solid State Physics Program

Program Leader: Prof. János Lendvai

Institute for Solid State Physics and Optics

Theoretical Solid State Physics

Budapest, 2012.

1. Introduction

In the last decades, due to significant technological development it became possible to examine small magnetic structures experimentally as well as theoretically. Nowadays, therefore, much energy is invested in the research of nano phase materials. From a theoretical point of view, these systems are interesting, because the low dimensional physics come to the front. From a practical point of view, these systems are important because the magnetic nano structures may be used in spin-devices and magnetic recording equipment. Behavior of magnetic nano structures on non magnetic surfaces is specially interesting, because the spin orbit coupling of both the host and the impurity can influence electron or magnetic structure in a fundamental way.

It is well known, that at surfaces of transition metals or semiconductors there are states, that form only on the surface, and do not exist in the bulk. These are often referred to as a surface state or surface resonance. Because of it's parabolic dispersion, the surface state can be regarded as a nearly free, two dimensional electron gas. This state plays a significant role in the case of semiconductor surface physics. Recently, there are several theoretical and experimental work on surface states at transition metal surfaces. On such surfaces, the spatial range (perpendicular to the surface) of a surface state is several layers. As it turns out, the surface state of the host plays a dominant role in the exchange interaction energy between surface magnetic impurities.

It is well known, that the exchange interaction between magnetic impurities in non magnetic bulk materials – the so called RKKY interaction – is an interaction that oscillates with the distance of the impurities between an anti-ferromagnetic or ferromagnetic ground state configuration. This interaction is mediated by the conduction electrons. The RKKY interaction decays like $1/R^3$, where R is the distance of the two impurities. The frequency of oscillation comes from the Fermi surface of the bulk host material. It was found that there is a similar oscillatory coupling between magnetic layers trough a stack of non-magnetic spacer layers. This interaction also oscillates and decays like $1/D^2$ where D is the thickness of non magnetic layer. The relative orientation of the magnetic moment of the magnetic layers depends on the sign of the interaction, the coupling can be ferromagnetic or anti-ferromagnetic. In this case the frequency of oscillation comes from the electronic structure of the non-magnetic spacer layer. Keeping these in mind, the question naturally arises, what were the interaction between surface impurities, and whether their behavior were similar? Such a research is obviously the first step towards the study of interaction between magnetic nano structures. The basic problem for such a study is to describe (or model) the electronic structure of the semi-infinite surface host. Therefor a comprehensive study of this problem is still missing. Using first-principles methods, this later difficulty can be solved quite elegantly, and with sufficient accuracy and in a material specific way. In this theses I attempted to give a a complete picture of interaction between surface impurities with a set of systematic calculations.

2. Methods

For the numeric calculations I used first principles electronic structure calculation within multiple scattering theory which enables the treatment of the semi-infinite host exactly. I calculated the Bloch spectral function in the full surface Brillouin zone to determine the dispersion of the surface state. I also implemented the calculation of the Bloch spectral function within the CPA theory for alloy surfaces, which enabled the calculation of the dispersion relation of surface states at surfaces of random substitutional alloys for the first time. One fundamental advantage of the method that the magnetic impurities could be embedded into the layers via a Dyson equation, and therefore, no super-cell approximation was necessary. Also, the calculations were based on the Dirac equation, fully taking into account the effect of spin-orbit coupling. Below I summarize the major results of the work.

3. Results and conclusions

1. I demonstrated numerically that at gold (110) surfaces there is anisotropic Rashba effect. Generally, the the Rashba splitting is thought to be isotropic and a function of spin-orbit coupling only. However, from the numerical calculations I concluded that the isotropic Rashba Hamiltonian does not give a correct description of the surface-state dispersion in all cases.

2. I implemented the calculation of the Bloch spectral function within the CPA theory for alloy surfaces, which enabled the calculation of the dispersion relation of surface states at surfaces of random substitutional alloys. I determined the dispersion relation of surface state at surfaces of Cu_xAu_{1-x} and Cu_xPd_{1-x} alloys and confirmed the existence of surface state in CPA theory.

3. I determined the exchange interaction between magnetic impurities with detailed numerical calculations. From theses calculations, I concluded that, where the surface states do exist and are occupied, they mediate the exchange interaction between the impurities. In this case the interaction is an oscillatory function of the distance between the impurities (R) and decays like $1/R^2$. The frequency of the oscillation comes from the Fermi vector of the surface state. At gold (111) surface there is two oscillation frequency, which is the consequence of the Rashba splitting of the surface state.

4. At copper (100) and gold (100) surfaces, where there is no occupied surface state, I found that there is no long range interaction. The interaction decays exponentially.

5. I analyzed the exchange interaction on surfaces of random substitutional alloys as well. On alloy surfaces I found an additional exponential decay of the interaction due to the disorder. At the surface of Cu_xAu_{1-x} alloys, due to the different spin orbit coupling of components, in the gold rich side the oscillation included two distinct frequencies. The oscillatory coupling between surface impurities could be observed in the entire concentration range. At the surface of Cu_xPd_{1-x} alloys, the situation is entirely different. Due to the closing of the Fermi neck with increasing Pd concentration, the interaction disappears as the surface state is destroyed. Surprisingly, in the palladium rich side, the oscillatory coupling can be observed again, albeit with a different type of decay and frequency.

6. I calculated the interaction of impurities on the surface Pt(111) as well, and obtained an oscillatory coupling without surface state in agreement with experiments. I found strong evidence, that this is due to the large induced moments in the platinum host. The frequency and the decay of the interaction is found to be the same as for RKKY interaction in bulk platinum. I calculated the platinum induced moments and demonstrated the role of the induced moments with a simple numerical model.

4. Publications

- E. Simon, A. Szilva, B. Újfalussy, B. Lazarovits, G. Zaránd and L. Szunyogh: Anisotropic Rashba splitting of surface states from the admixture of bulk states:

Relativistic ab initio calculations and kp perturbation theory, Phys. Rev. B; **81**, 235438 (2010)

- E. Simon, B. Ujfalussy, B. Lazarovits, A. Szilva, L. Szunyogh, G.M. Stocks: Exchange interaction between magnetic adatoms on surfaces of noble metals, Phys. Rev. B **83**, 224416 (2011)
- E. Simon, B. Újfalussy, A. Szilva and L. Szunyogh; Anisotropy of exchange interactions between impurities on Cu(110) surface, Journal of Physics: Conference Series; 200, 032067 (2010)
- E. Simon, B. Lazarovits, L. Szunyogh, and B. Újfalussy ; Ab initio investigation of RKKY interaction on metallic surfaces; Philosophical Magazine B; 88, 2667-2682 (2008)
- Sz. Vajna, E. Simon, A. Szilva, K. Palotas, B. Újfalussy, L. Szunyogh: Higher-order contributions to the Rashba-Bychkov effect with application to Bi/Ag(111) surface alloy (arxiv:1110.3953)
- B. Újfalussy, E. Simon: Impurity exchange on alloy surfaces (to be published)

Other publications:

- I. Bakonyi, E. Simon, B. G. Tóth, L. Péter, and L. F. Kiss; Giant magneto resistance in electrodeposited Co-Cu/Cu multilayers: Origin of the absence of oscillatory behavior; Phys. Rev. B; **79**,174421 (2009)
- Cziráki Á, Péter L, Weihnacht V, Tóth J, Simon E, Pádár J, Pogány L, Schneider CM, Gemming T, Wetzig K, Tichy G, Bakonyi I; Structure and giant magneto resistance behaviour of Co-Cu/Cu multilayers electrodeposited under various deposition conditions; J. Nanosci. Nanotechnol.; **6**, 2000-2012 (2006)
- Bakonyi I, Simon E, Péter L; Az óriás mágneses ellenállás felfedezése (1988)- a spintronika nyitánya (in Hungarian); Fizikai Szemle, LVIII. évfolyam 2. szám (február), 41-45 (2008)
- Bakonyi I, Simon E, Péter L; Mágneses ellenállás ferromágneses fémekben és mágneses nanoszerkezetekben (in Hungarian); Fizikai Szemle LVIII. évfolyam 3. szám (március), 93-98 (2008)